Condition Estimation by Means of the Power Method

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Abstract

We estimate the condition number of a matrix by applying the Power Method, that is essentially a sequence of matrix-by-vector multiplications, similarly to the Lanczos-based estimators.

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Condition estimation is fundamental task for for numerical matrix computations, supported by a number of effective algorithms [GL96, Sections 2.3.2, 2.3.3, 3.5.4, 12.5], [H02, Chapter 15], and [S98, Section 5.3], which rely on solving linear systems of equations or orthogonalization. These techniques, however, are not friendly to sparse and structured inputs of large sizes, and this motivates creating alternative methods, employing matrix-by-vector multiplications instead. We describe such a simple estimator based on the Power Method, which is similar to the Lanczos-based estimators.

Assume a real symmetric nonnegative definite $n \times n$ matrix S and apply the Power Iteration

$$\mathbf{v}_k = S^k\mathbf{v} = S\mathbf{v}_{k-1},\ k = 1, 2, \dots \tag{1}$$

for a random vector $\mathbf{v} = \mathbf{v}_0$ to approximate the largest eigenvalue $\lambda = \lambda(S)$ of the matrix S by the Rayleigh quotients $q_i = \mathbf{v}_k^T S\mathbf{v}_k/\mathbf{v}_k^T\mathbf{v}_k$. Using the Power Method for the norm estimation was proposed in [B74]. The paper [D83] proved that $q_k \le \lambda\, \theta q_k$ with a probability at least $1-0.8\theta^{-k/2}n^{1/2}$ for any scalar $\theta > 1$. This estimate defines a stopping criterion for the iteration, and heuristically one can also stop where $q_i/q_{i-1} \approx 1$ or $||S\mathbf{v}_i - q_i\mathbf{v}_i||/(|q_i)|\ ||\mathbf{v}_i||) \le t$ for a fixed tolerance t. Instead of the Rayleigh quotients one can use the simple quotients $s_i = \mathbf{e}_i^T S\mathbf{v}_k/\mathbf{e}_i^T\mathbf{v}_k$ for the ith coordinate vectors $\mathbf{e}_i$ and fixed or random integers $i = i(k)$, $1 \le i \le n$ (cf. [BGP04], [PQZC]), [PZ11]).

Now assume an $m \times n$ matrix A for $m \ge n$, let $\sigma_j(A)$ denote its jth largest singlular value, and seek a crude estimates for $\sigma_1(A)$ and $\sigma_n(A)$, e.g., to decide whether the matrix is well conditioned. One can approximate the smallest eigenvalue of the matrix A^TA, equal to $\sigma_n^2(A)$, by applying the Power Method to the inverse matrix $(A^TA)^{-1}$ (cf.[H02, Chapter 15]), but this involves solving linear systems of equations, and we can avoid that as follows.

Apply the power iteration (1) to the matrix $S = A^TA$ to compute a close upper bound σ_+^2 on $\lambda(S) = ||A||^2 = \sigma_1^2(A)$. Then apply the power iteration (1) to the matrix $B = \sigma_+^2 I - A^TA$ to compute an approximation λ_+ to its largest eigenvalue and then obtain $\sigma_+^2 - \lambda_+ \approx \sigma_n^2(A)$. An even superior alternative is to approximate both largest and smallest eigenvalues of A^TA by applying the Lanczos algorithm, which converges faster than the Power Method [KW92].

For $m \le n$ apply the same techniques to the matrix AA^T.

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